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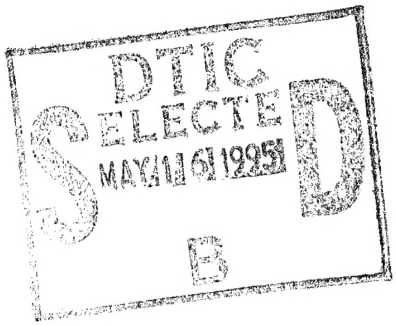
SURVEY OF HIGHLY STRUCTURED, GENERAL PURPOSE, STEADY STATE CHEMICAL PROCESS SIMULATION SOFTWARE PACKAGES

Stuart Levy and Raymond Goldstein



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13. ABSTRACT (Maximum 200 words)

As a FY 93 task under the SERDP Project to Develop Clean, Agile, Manufacturing Technology for PEP Materials, a survey was conducted which evaluated features and capabilities of what are felt to be the three leading PC-based chemical process flowsheet simulation software packages commercially available today–PRO/II, ASPEN PLUS, AND CHEMCAD. A list of 24 characteristics/attributes common to each package (including cost) was developed and used a a framework around which to gather information. Information was obtained from the open literature, as well as directly from the software vendors through technical manuals, office visits, phone conversations, and demonstrations by technical sales personnel. Each feature was described in narrative form and an attempt was then made to compare and rate each of the three packages using a structured evaluation matrix. Based on this methodolgy, ASPEN PLUS was seen to have the most highly rated capabilities. However, when cost was factored in, CHEMCAD was shown to give the best value for the money. With regard to incorporating as a detailed process simulator within a larger life cycle modeling system, each of the packages would function acceptably assuming a file linking program was in existence to provide a structured data interface. In this regard, PRO/II might cause some unique problems because of its functional dependency on a Windows environment and CHEMCAD might offer some advantage because of its underlying C code foundation.

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INTRODUCTION

Recent events suggest that the future of munitions production will be characterized by low requirements, lean budgets, and reduced allocation of resources. Diminished funding is also anticipated for research and development (R&D) related to the Army's munitions manufacturing base. As stated by W. Brad Bergmann, II, Director of Manufacturing Modernization, Office of the Assistant Secretary of Defense (Pollution and Logistics) at the 5th INFAC Coalition Meeting in October 1991, "DoD is facing an era of continually decreasing budgets. We will simply have to make do with less. We will have to use what funds we get as efficiently and as effectively as possible....The new systems we do buy will require advanced technology--product and production technology." In such periods of reduced requirements and resources, a premium is placed on production efficiency and product quality which, in turn, demands that optimization of both plant design and operating strategy be considered and enforced. Mathematical modeling and computer simulation provide the tools by which such improvements can be carried out and implemented in a structured, controlled, cost effective way which places neither personnel nor facilities at risk.

In conjunction with optimized process design and operation (which inherently lead to improvements in efficiency, flexibility, and agility), there is currently a major focus on minimization of environmental impact during munitions production. In this regard, the emphasis is on pollution prevention rather than end-of-pipe treatment. Pollution prevention is accomplished by running each unit operation within the process, as close as possible to its minimum pollution point within technology constraints and economic considerations. The locus of points of minimum pollution at a given outlay of capital defines the so-called Pareto curve and is the sought after objective for process operation.

In keeping with this philosophy, a major effort is now underway within the U. S. Government munitions production establishment to create clean, agile factories. Computer simulation will play a big part in this undertaking. In February 1993, a joint Department of Defense/Department of Energy (DoD/DoE) project funded under the SERDP umbrella was approved for execution over a 5 yr period. The project objective is to develop integrated product/process development (IPPD) technologies and tools to demonstrate concepts for reconfiguring existing PEP life-cycle facilities into clean, agile operations that will function economically with total life-cycle wastes reduced by 90%. Project tasking is divided into two functional areas: technology development and/or evaluation and computer model development. It is in support of the latter that the work documented in this report has been conducted.

Under the SERDP Agile Project, a life-cycle analysis software system is being developed based on a two-tiered approach. The top level will consist of a data driven life cycle inventory model in which processes are viewed at the building level and relationships between material inputs and outputs are essentially constant and

established, based on archived process data. The second level will involve detailed process models which are unit operations driven and implemented using a highly structured, general purpose process simulation software package. Detailed simulation will be conducted in order to update the input/output relationships in the top level model whenever significant excursions from the base point are made; detailed simulation will also provide insight into the performance of proposed alternative technologies which may be suggested during the course of life-cycle improvement analyses.

In order to insure use of state-of-the-art methodology, the requirement to conduct a survey of commercially available, highly structured, general purpose, PC-based chemical process simulation software packages was included in the Agile Project scope of work. ASPEN PLUS, CHEMCAD, and PRO/II were viewed as the top three process simulators on the market and selected for evaluation. The features of each are described in the following pages and a comparative analysis is made. As a starting point and to set the tone of this report, the words of John Baldwin, Process Engineering Manager at M.W. Kellogg, Chairman of the Process Data Exchange Institute of AIChE and noted simulation expert are offered: "Most steady state simulation packages are very similar. The differences in capabilities are in the twists that give one program an advantage over another in predicting a particular application. However, the current crop of simulators has been updated to address identified weaknesses so that these lines of differentiation have become even less defined."

FEATURES OF CANDIDATE SOFTWARE PACKAGES

A list of 24 characteristics/attributes common to each of the three candidate software packages was established (table 1) and used as a framework around which to gather the information for the survey.

Purchase Cost and/or Licensing Requirements

Of the three simulation software systems evaluated, two are available on a lease-only basis while one can be purchased. The vendor's who lease their software contend that this is the only way to insure that the latest features are in use, and that outmoded obsolete versions do not proliferate, which would be detrimental to the software's quality reputation. Leasing is also a way for the vendors to reduce their customer support burden since questions related only to the current version would have to be addressed.

Purchasing involves a one-time cost for the software package, followed by optional annual upgrades or so-called maintenance charges. Paying for maintenance guarantees the user all improvements and enhancements as they become available. However, if the user's simulation requirements are satisfied at some point, it may not

be of any subsequent benefit to continue upgrading for features which are either not applicable to the user's environment or simply not wanted. Discontinuing maintenance still leaves the user with a viable (although potentially outmoded) simulation package, whereas terminating a lease results in loss of the software. There is no clear cut right choice and a lease or buy decision would have to be based on the user's own perception of cost versus performance.

PRO/II

PRO/II can be obtained only on a leasing basis. A new release of PRO/II was available at the end of the summer of 1994 and cost $25,000 for the first year. As a special introductory offer for those who commit to lease the new version prior to its release date, a 70% reduction in cost for the next 2 yrs is offered resulting in a $40,000 total cost for the initial 3 yr contract. After that, the leasing fee would return to the prevailing rate. A discount is also available for multiple users. Customer support service is obtainable as part of the leasing arrangement.

ASPEN PLUS

ASPEN PLUS is also available only on a leasing basis. The leasing fee on a yearly basis is $24,000 for a single user, $47,000 for two users, $61,000 for three users, and $75,000 for four users. Each user would have their own stand-alone copy of the software. A discount of 25% is offered if leased on a 3 yr basis. Thus, the fee for one user on a 3 yr contract would be $55,250. The cost of training is included in the rental fee.

CHEMCAD

CHEMCAD can be purchased at a cost of $11,500. The purchase price includes 1 yr of free updates. Subsequent annual updates can be purchased at the user's option at a cost of $3,000.

Number and Type of Different Unit Operation Models

The set of unit operation models is one of the key building blocks upon which a simulation software system is based. In essence, it determines what type of and to what level a chemical plant can be simulated.

It should be noted that, for a given class of unit operation, one simulation package may have more models than another. However, that does not necessarily mean it has more simulation capability because the code in one system's software module may be equivalent to one or more modules of the other.

PRO/II

There are 35 unit operation models grouped in five classes including:

Generalized flowsheet (8 models): flash, valve, compressor, expander, pump, pipe, mixer, splitter

Distillation (9 models): inside/out algorithm, sure algorithm, chemdist algorithm, electrolyte, liquid/liquid extractor, batch, shortcut, packed columns, tray sizing/rating

Heat exchanger (5 models): rigorous (shell and tube), simplified, LNG (cold box), zones analysis, heating/cooling curves

Reactor (7 models): conversion/equilibrium reactor, plug flow, continuous stirred tank, in-line FORTRAN kinetics, Gibbs free energy minimization, shift and methanization

Solids handling (6 models): crystallizer, dissolver, countercurrent decanter, centrifuge, rotary filter, dryer

ASPEN PLUS

There are 41 unit operation models grouped in eight classes as follows:

Simple stream handling (5 models): general mixer, flow splitter, substream splitter, component splitter, two-product separator

Flash separators (2 models): two-phase, three phase

Heaters and heat exchangers (3 models): general process heater, heat exchanger, multistream heat exchanger

Multistage separation (8 models): rigorous fractionation, multiple column rigorous fractionation, rigorous absorption, rigorous extraction, shortcut distillation [3 models]

Reactors (7 models): yield-based, stoichiometric, continuous stirred-tank, plug flow, two-phase chemical equilibrium, general phase and chemical equilibrium, batch

Pumps and compressors (3 models): pump/slurry pump, single-stage compressor/expander, multistage compressor/expander

Solids handling (11 models): cyclone, electrostatic precipitator, fabric filter, venturi scrubber, crusher, screen/classifier, hydrocyclone, rotary drum filter, filtering centrifuge, solids washer, counter-current decanter

Stream manipulators (2 models): multiplier and duplicator

CHEMCAD

There are 38 unit operation models grouped in eight classes as follows :

Reactors (4 models): stoichiometric, equilibrium, Gibbs, kinetic (plug flow or continuous stirred tank)

Solids handling (13 models): crystallizer, centrifugal filter, cyclone, washer, venturi scrubber, baghouse filter, screen, hydrocyclone, vacuum filter, electrostatic precipitator, dryer, sedimentation separator, crusher or grinder

Pumps and compressors (3 models): compressor(adiabatic and polytropic), liquid pump, expander

Multistage separator (5 models): rigorous fractionation(simultaneous corrections), rigorous fractionation(inside/out), short-cut distillation, complex tower, liquid/liquid extraction

Flash (2 models): multipurpose flash, liquid-liquid-vapor 3 phase flash

Simple stream handler (7 models): component separator, stream divider, stream mixer, phase generator, pipeline sizing/rating, valve

Heater and heat exchangers (3 models): fired heater, multistream heat exchanger, LNG heat exchanger

Feedback/feedforward controller (1 model)

Extent of Detail in Unit Operation Models

It would not be possible, nor is it felt desirable, to provide in this report a detailed description of each unit operation model. In general, the level of detail and computational depth upon which unit operation models are based is similar for each of the three simulation packages evaluated. To illustrate this, as well as provide some basis for comparison, a rigorous distillation module and a Gibbs reactor have been selected as typical examples of unit operation modules.

PRO/II

Rigorous Distillation. All of the distillation algorithms in PRO/II are rigorous equilibrium stage models. Each model solves the heat and material balances and vapor liquid equilibrium equations. The features available include pumparounds, five condenser types, and generalized specifications.

PRO/II uses the inside/out (I/O) algorithm for most modeling. This algorithm is based on a method developed by R.A. Russel in 1983. The I/O algorithm can be used to solve most refinery problems and usually converges the fastest compared to other distillation algorithms.

The I/O algorithm contains a number of novel features which contribute to its excellent convergence characteristics. The algorithm is partitioned into an inner and outer loop. In the inner loop, the heat, material, and design specifications are solved. Simple thermodynamic models for enthalpy and vapor liquid equilibrium (VLE) K-values are used in the inner loop. This along with the form of the simple model and the choice of primitive variables, allows the inner loop to be solved quickly and reliably. In the outer loop, the simple thermodynamic model parameters are updated based on the new compositions and the results of rigorous thermodynamic calculations. When the rigorously computed enthalpies and K-values match those of the simple thermodynamic models, and the design specifications are met, the algorithm is solved.

Inner Loop. The primitive variables in the inner loop are the stripping factors and sidestream withdrawal factors. The inner loop equations are the stage enthalpy balances and the design specifications.

The system of equations is solved using the Newton-Raphson method. The first Jacobian matrix is obtained by finite difference approximation. This Jacobian is then inverted, and at subsequent iterations the inverse Jacobian is updated using Broyden's method.

To evaluate errors in the enthalpy and specification equations for a given set of stripping factors, the component flows and stage temperatures must be computed for the given stripping factors and simple model parameters.

Outer Loop. The outer loop in the I/O algorithm updates the simple thermodynamic model parameters and checks for convergence. In the inner loop, the distillation equations are solved for the current simple thermodynamic models. The convergence check in the outer loop therefore compares the rigorously computed enthalpies and VLE K-values from the new compositions resulting from the inner loop calculations.

The simple K-values can be calculated very quickly for a given temperature. Also, once new molar flows are computed in the inner loop, a new bubble point temperature can be easily computed. Once the molar flows are computed, the mole fractions are obtained.

ASPEN PLUS

Rigorous distillation in ASPEN PLUS is based on a variation of the I/O algorithm called RADFRAC. RADFRAC is a rigorous model for all types of fractionation including absorption, reboiled absorption, stripping, reboiled stripping, and extractive, azeotropic, and three-phase distillation, in addition to ordinary distillation. RADFRAC is suitable for both narrow-boiling and wide-boiling systems, systems exhibiting strong phase nonideality, and systems where equilibrium and/or rate-controlled chemical reactions occur. RADFRAC can be used for both rating and design calculations. Although equilibrium stages are assumed, either Murphree or vaporization efficiencies can be specified.

Convergence Parameters. The RADFRAC algorithm consists of two nested iteration loops. The K-value and enthalpy models specified by the user are evaluated only in the outside loop to determine parameters of simplified local models. In RADFRAC, a choice can be made for a non-ideal system in which case a composition dependence is introduced into the local models. The local model parameters are the outside loop iteration variables. The outside loop is converged when the changes of the outside loop iterations variables are sufficiently small from one iteration to another. Convergence is promoted using a combination of the bounded Wegstein method with the Broyden quasi-Newton method for the selected variables.

Additional features of the ASPEN PLUS I/O algorithm include:

- Integration of new simple models to enhance the local representation of physical properties, resulting in faster and more reliable convergence.
- Coupling of Newton's method with the I/O algorithm to enhance performance for highly non-ideal, electrolytic, and reactive systems.
- Use of the differential homotopy continuation method and Powell's dogleg strategy to promote convergence stability.
- Use of nonlinear optimization techniques for handling design specification convergence, to ensure column solutions when specifications are infeasible.

- Use of the Gibbs free energy minimization technique for the liquid-liquid phase split calculations when modeling three-phase systems, to avoid convergence to incorrect solutions.

CHEMCAD

Like PRO/II and ASPEN PLUS, CHEMCAD uses a computational scheme based on the I/O algorithm. It is called TOWR and is a rigorous multi-stage vapor-liquid-liquid equilibrium module which simulates any single column calculation including distillation columns, absorbers, reboiled absorbers, and strippers. Side products and side heater/coolers can also be modeled rigorously by TOWR. TOWR handles columns with a maximum of 100 stages, five feed streams, and four side products. There is no limit on the number of TOWRs in a flow sheet.

TOWR offers a variety of specifications which makes it very flexible to use. You can specify condenser, reboiler, or tray conditions. Specifications, such as total mole flow rate, heat duty, reflux ratio, boil-up ratio, temperature, mole fraction, recovery fraction, component flow rate, V/L ratio, mass flow rate, volumetric flow rate, mass fraction, flow ratio of two components, gravity, and molecular weight of products are allowed in TOWR.

Algorithms. Tower uses an enhanced I/O algorithm to simulate the tray to tray calculations. Basically, the outside loop sets up a local, simple K-value and enthalpy model to be used in inside loop calculations. The inside loop does most of the mass-energy-equilibrium calculations based on simplified K-value and enthaply model created by the outside loop to meet the MESH equations and the user specifications. When the inside loop converges, control returns to the outside loop which then updates the simple K-value and enthalpy model by using the results of rigorous K and enthaply calculations. When the simple model matches the rigorous model to the desired tolerance, the outside loop is defined as converged. If not, a new simple K and enthalpy model is generated by the outside loop and the inside loop calculation repeats. When both inside and outside loop converge, the tower calculation is finished.

PRO/II

Gibbs Reactor. The Gibbs reactor computes the distribution of products and reactants that is expected at chemical equilibrium for a system of reactions and species. The method of Free Energy Minimization, by White, Johnson, and Dantzig with modifications by Oliver et al. is used. The objective of calculating equilibrium composition is to know the maximum obtainable yield or to operate under the conditions away from equilibrium. The advantage of using the free energy minimization over the traditional Arrhenius equilibrium constant method lies in the fact that individual stoichiometric equilibria need not be considered. Rather, all the possible species

are noted, and the distribution of these species is established using a general mathematical technique to give minimum free energy for the system. The mathematical procedure used requires no prior knowledge of the chemistry of the system, nor does it require accurate first guesses, although reasonable accurate guesses reduce computing time. The basic outline of the method is as follows:

- Develop expressions for the free energy of the system
- An expression is written for the free energy of a mixture of assumed composition
- The free energy of the equilibrium mixture (whose composition is unknown) is expressed in terms of the known mixture and of unknown increments which represent the changes necessary to bring the assumed initial compositions to the final equilibrium compositions. The expressions used involve the first two terms of a Taylor series and is thus termed a quadratic approximation. The magnitude of these unknown changes or, more precisely, the revised values for the species, are to be found.
- The expanded function (the quadratic approximation to the minimum free energy) is minimized subject to the mass-balance constraints using the technique of Lagrange Multipliers.
- These manipulations yield a system of m + p + 1 simultaneous equations in as many unknowns, where m is the number of elements and p is the number of condensed species.
- The procedure is repeated, until convergence is obtained, i.e., two successive composition sets agree to within the accuracy desired. At this point, the free energy of the system is a minimum.

ASPEN PLUS

RGIBBS is a reactor model which can be used for single-phase chemical equilibrium; simultaneous phase and chemical equilibrium; or phase equilibrium without chemical reactions, particularly for multiple liquid phases. RGIBBS calculates equilibrium by Gibbs energy minimizations with phase splitting. The reaction stoichiometry does need to be specified. RGIBBS can also be used when the system does not reach complete equilibrium. The equilibrium can be restricted by specifying the

extent of a reaction, the temperature approach to equilibrium, or the amount or fraction of a component that does not react. RGIBBS can be used to compute single phase (vapor or liquid) chemical equilibrium, phase equilibrium (an optional vapor and any number of liquid phases with no chemical reactions or simultaneous phase), and chemical equilibrium.

Chemical Equilibrium. One must specify a list of possible products. RGIBBS finds the distribution of the specified products that gives the minimum Gibbs free energy while satisfying atom balances. If the system contains one or more slow reactions that do not reach equilibrium, a restricted chemical equilibrium can be performed. If phase equilibrium is not also considered, one must specify whether the single phase is vapor or liquid.

Phase Equilibrium. RGIBBS automatically determines the number of phases present, up to a maximum that the user specifies. Whether or not the single phase is considered, must also be specified.

Restricted Chemical Equilibrium. Several different types of specifications are permitted. If the molar extent of a reaction is known, its value can be specified. A temperature approach to chemical equilibrium can be specified for an individual reaction. When a temperature approach is specified for a reaction, the chemical equilibrium constant is evaluated at the temperature T + DT, where T is the actual reactor temperature specified by the user and DT is the desired temperature approach. The outlet amount of any of the components can be fixed, either as total moles or as a percentage of the feed. If either the molar extent of a reaction or the temperature approach for an individual reaction is specified, then you must supply the stoichiometry for a set of linearly independent reactions involving all components present in the system.

CHEMCAD

The GIBBS reactor model may be used to simulate reactors for the purpose of heat and material balances. Product rates, compositions, and thermal conditions are calculated by the minimization of Gibbs free energy, subject to an overall mass balance. All components in the component list are considered in the Gibbs free energy minimization calculation unless specifically excluded (identified as inert).

For standard data base components, the minimum information required by the Gibbs reactor is the identity of the feed and product streams. Temperature and/or pressure may be set, if different from those derived from the feed stream(s). No reaction stoichiometry is required.

The reactor can be operated with a single liquid or vapor phase specified or as a mixed phase reactor. It may be operated isothermally at a specified temperature, or at the feed temperature. Heat may be added or removed and temperature limits may be imposed.

For user-supplied or pseudo-components, the free energy of formation, molecular weight, and heat capacity must be supplied. For solid components, the free energy of formation, the heat of formation, molecular weight, and heat capacity must be present in the data base.

Several overall constraints may be imposed on the reaction. The temperature approach to chemical equilibrium of the entire reacting system can be specified. In this case, the chemical equilibrium is determined at T + DT, while the properties are computed at T, where T is the reactor temperature and DT is the approach to chemical equilibrium.

Methods. With free energy minimization, individual equilibria are not considered as such. Rather, the possible reaction species are noted, and the distribution of these species is established using a general mathematical technique to give a minimum free energy for the system. Thus, for any reaction system, all important species are noted and the solution is carried out without prior knowledge of the chemistry of the system. The solution so achieved will satisfy all expected equilibria and be accurate within the limits of the thermodynamic data. Basically, free energy minimization is accomplished through the execution of a stepwise procedure. First an expression for the free energy of the system is developed by writing an expression for the free energy of a mixture of assumed composition. The free energy of the equilibrium mixture (composition unknown) is expressed in terms of the assumed mixture of unknown increments which represent the changes needed to bring the assumed mixture composition to the final equilibrium composition. The expanded function (i.e., quadratic approximations) is minimized, subject to mass balance constraints by using Lagrange multipliers. As a result of the manipulations involved, a system of linear simultaneous equations is obtained in as many unknowns. When solved, the system yields a new composition that represents a new approximation of the composition which gives minimum free energy. The procedure is repeated until the calculated and prior compositions are within acceptable agreement. At this point, the free energy of the system is at a minimum.

Quality and Features of the Graphical User Interface

In look and feel, the graphical user interface (GUI) of PRO/II, ASPEN, and CHEMCAD are similar. To construct a process model through the GUI, icons are selected for each unit operation or equipment item and placed on a flow sheet area of the screen. The equipment icons of the three companies are similar since standard

symbols are used to specify equipment and instrumentation. Using a mouse, lines are drawn between each equipment icon to establish streams. As the flow sheet is constructed, pointing and clicking on an equipment item or stream opens up a data entry window through which various required data and parameters are input. Data banks of component information are available; component data is automatically brought into the simulation when a component is selected either by component number from a list or by chemical name or formula.

While both ASPEN PLUS and CHEMCAD have a Windows look and feel, only PRO/II is implemented as a true Windows application. At the time of this writing ASPEN PLUS was planning to release a Windows version within the next year.

Ease of Simulation Creation

PRO/II

Creating a simulation is accomplished through the GUI. The GUI enables the user to draw the process flow diagram and enter data directly. To create a process flow sheet, the user selects an icon that represents a unit operation and places it on the screen. This process is repeated until all the unit operations of the process appear on the screen. Next, the unit operations icons are connected to form streams. Engineering units, component names, stream properties, and equipment data and parameters are entered from lists and screen menus. The simulation may be run interactively, adding one unit operation at a time, until the complete model simulation is achieved. Output may be presented in graphical or tabular form.

Simulation is made easier through the use of forms, lists, menus, expert systems, automatic flow sheet drawing, and intelligent output review through plots, graphs, and automatic case compare.

ASPEN PLUS

ASPEN PLUS has a graphical user interface called ModelManager that allows the user to draw the process flow diagram and enter data directly. Model-Manager has an expert system that guides the user in entering data on the many screens. The screens have context sensitive help which define the information required. The expert system prompts the user when there is too little, or too much information, or complete information on the screen. If the user is uncertain as to what step to take next upon entering information into the system, he simply strikes the "next" key, which triggers the expert system to advise the user what steps to take next in completing the simulation. When options are to be selected, a complete list of options is provided and context sensitive help is available to explain the options. The expert system guides the user in each step of the model building. The model is assembled in blocks and each block may be run interactively and tested separately from the other blocks.

The nine procedural steps in creating a flow sheet model include:

1. Define the process flowsheet to be modeled and the purpose of the model

2. Select the units of measurement for input data and output reports

3. Specify what chemical components will be present in the streams of the flowsheet

4. Specify the methods and models to be used for calculating physical properties

5. Break the process flowsheet into unit operation (equipment) blocks and choose an appropriate model for each block

6. Define the feed streams to the process

7. Specify the performance of each unit operation block to represent the design and operating conditions of the process

8. Impose any design specifications

9. Set up sensitivity analyses or case studies

This procedure represents the general steps required for creating a process flowsheet. To carry out these steps using the ModelManager GUI, the user would first select a unit operation from a list of operations and place its icon on the screen. He would repeat this procedure until all the unit operations of the process were placed. The next step would be to connect the unit operations on the screen to form streams. Next the engineering units would be selected from a list. The chemical components are chosen from a list in the data bank by specifying its name or chemical formula. Next, the thermodynamic requirements are chosen from a list. For each stream, its temperature, pressure, flow, and other data are specified. For each item of equipment or unit operation, all the pertinent data necessary for its operation is entered on the screen. The simulation may be run interactively, adding one block or unit operation at a time, testing the model with each addition until full simulation is achieved. The output may be presented in tabular or graphical form. The validity of the model may be established by comparing the output of the model with the real data of the process.

CHEMCAD

CHEMCAD employs a graphical user interface that allows the user to draw the process flow diagram directly on the screen, and enter engineering data and equipment parameters through the use of menus or screens. The input data and graphics are totally integrated. The flow diagram is always on the screen for immediate reference. Menus guide one through the problem solving process, and on-line help is available at any time.

There are five procedural steps involved in creating a process model:

1. Setting up a problem. This involves using the job selection and accounting option to specify a code for a new flow sheet.

2. Creating a flowsheet. In this step the flowsheet/PFD graphics option is used to arrange unit operations and streams. The topology associated with the flowsheet is automatically transferred to subsequent steps.

3. Specifying engineering data. All engineering data required for performing heat and material balances is loaded interactively through templates which are available on pull-down menus. The following data may be loaded:

- Feed intermediate, and product stream components
- The K value methods to be used for equilibrium calculations
- The H value methods to be used for enthalpy calculations
- Engineering units to be used for temperature, pressure, etc
- Feed stream compositions
- Equipment parameters for each unit operation

4. Performing the simulation. This is accomplished by invoking the interactive simulator RUN command to perform the following steps:

- Check input data for errors
- Perform all engineering unit conversions
- Regress equilibrium and vapor pressure data

- Use distillation curve data to create hydrocarbon pseudo-components
- Estimate the physical properties of hydrocarbon pseudo-components and all chemical compounds whose physical properties are not specified in the data base
- Calculate dew points, bubble points, and a host of other derived physical properties
- Perform steady-state heat and material balances for the whole flow sheet

5. Viewing and printing the results. The results can be displayed on the screen or printer in tabular form or can be displayed as X-Y plots.

CHEMCAD also has a feature called COACH, which is an option in the control menu that coaches you through the above steps for creating a simulation. It has hand-holding options that display help windows explaining each step and then lets you perform that step.

Like ASPEN PLUS and PRO/II, the user follows an almost identical procedure to create the process flow sheet. A unit operation is first selected from a menu of icons and with the use of a mouse placed on the screen. This procedure is continued until the flow sheet is complete. The mouse is then used to draw connecting lines between icons. These lines represent process streams. With the use of menus, screens and lists, the user enters engineering units, components id's and properties, stream properties, and calculation procedures. He may run the simulation interactively, adding one unit at a time until the simulation is complete. The output may be presented in tabular or graphical form.

User Friendliness and Expected Learning Curve

ASPEN PLUS, PRO/II, AND CHEMCAD are all user friendly. Each has some form of data input consistency and completeness checking, which informs the user when erroneous or incomplete data has been entered in the process of defining a model. The user is also prompted to supply specific data elements which are characteristic of the model being structured. ASPEN PLUS is the most highly evolved in this area with its ModelManager which it advertises as an expert system running within the GUI. ASPEN PLUS also has a "next" key to help the user navigate through the simulation. CHEMCAD has COACH, similar to the "next" key of ASPEN PLUS, which helps guide the user through all the simulation steps. All have context sensitive help screens.

The expected learning curve depends on the background of the user. A computer literate chemical engineer, after taking a vendor-offered introductory training course(3-5 days), could probably reach a minimum proficiency level in about two weeks.

Open Architecture

Open architecture addresses the ability of a software package to enable writing user-defined custom models which can then be linked to the object code as well as the ability to seamlessly interface with third party software.

PRO/II

The new version of PRO/II is a 100% Windows application. This is an advantage since it means that PRO/II users can easily navigate through file manipulation procedures in Windows to port output data from PRO/II simulations to spreadsheets, database programs, or any other programs that run under a Windows environment. Users can also develop their own calculation methods in FORTRAN and link them into PRO/II. The user can access the standard utilities (i.e. flash calculations, property predictions) available in PRO/II, and use them in their own calculation blocks.

ASPEN PLUS

ASPEN PLUS directly interfaces with most commercial spreadsheet programs, with major heat exchanger programs such as HTFS, with AutoCAD, with plant design systems such as PASCE and Intergraph/PDS, and with the PRODABAS engineering data base. ASPEN PLUS has in-line FORTRAN, user models to facilitate customization.

ASPEN PLUS also has a summary file retrieval tool kit which allows building of custom interfaces between ASPEN PLUS and other programs. The summary file is a compact ASCII file that contains all the results of a simulation. The tool kit provides a set of FORTRAN subroutines for retrieving data from the summary files for use in other programs.

CHEMCAD

CHEMCAD interfaces directly to Lotus 1-2-3 and AutoCad. By making appropriate menu choices, CHEMCAD's graphics can be dumped directly into AutoCad's PFX format and then loaded into AutoCad. Similarly, tabular output reports from the simulation can be saved as a LOTUS PRN file. CHEMCAD also allows user-defined custom models. These can be written either in FORTRAN or in C/C++. Chemstations suggest C/C++ be used over FORTRAN because CHEMCAD III is written in C (and assembler); however with a specific compiler (Watcom) and Pharlap's 386/DOS Extender, FORTRAN models can be seamlessly incorporated.

Extent of Vendor-Supplied Physical Properties Data Bases and Ability to Link New Data Bases and/or Compounds

PRO/II

PRO/II contains three data bases for pure component physical properties, two for mixtures as well as various data bases for binary interaction parameters. The pure components data bases include 1,600 pure components (incorporating the DIPPR library), a solids properties data base, and an electrolyte data base.

The two mixture data bases have more than 3,000 regressed parameters on-line and special data packages for alcohol, glycol, and sour water systems.

The binary interaction data bases contain parameters for various equations of state and other rules for physical property estimation. Included are parameters for S-R-K, P-R, Huron-Vidal Mixing Rule, Panagiotopoulos & Reid Mixing Rule, Simsci Mixing Rule, BWRS, UNIQUAC, NRTL-8 Coefficient Form, Henry's Law for Non-Condensables, Heat of Mixing, and Hayden-O'Connell.

ASPEN PLUS

ASPEN PLUS contains six data bases for physical properties of pure components, two for binary interaction parameters and also provides interfaces to DECHEMA (phase equilibrium data base) and CSIRO, a data base of parameters for 3,000 organic and inorganic substances.

The pure component physical properties data bases include ASPENCD with parameters for 500 compounds, Barin with information on 2,400 inorganic and organic substances used in solute handling applications, DIPPR with data for 1117 compounds, and data bases for 121 solid species and 260 ionic species and molecular solutes.

The two binary interactive data bases include information on Henry's Constant for 61 species in aqueous solutions and parameters for various equations of state models including S-R-K, P-R, L-K-P, BWR-Lee-Starling, and Hayden-O'Connell.

CHEMCAD

CHEMCAD maintains a standard data base for physical properties of 1,540 pure components, and a data base of about 22,000 pairs of binary interaction parameters for use with the NRTL, UNIQUAC, Margules, Wilson, and Van Laar activity coefficient methods. A data base for binary interaction parameters (BIPs) for mixtures that use activity coefficient methods is also included.

CHEMCAD provides a data base for solving a significant set of problems involving electrolyte and nonelectrolyte species in a variety of unit operations as well as a data base for vapor phase association effects. This affects the K-value calculation when using activity coefficient methods.

CHEMCAD provides an interface to corporate data bases which allows specific proprietary data to be used if available.

PRO/II, ASPEN PLUS, and CHEMCAD all have the ability to add new physical properties for existing components as well as new components to their data banks.

Number and Types of Thermodynamic and Transport Property Models

Thermodynamic/transport property packages provide a variety of options to generate K-values, enthalpy, entropy, density, molar volume, vapor pressure, viscosity, thermal conductivity, and surface tension for process streams.

PRO/II

There are 12 classes of models including:

K-Value methods (15 models)

Activity coefficients (8 models)

Equations of state (13 models)

Three phase equilibrium models

Heat of mixing models

Electrolyte models

Mixing models

Liquid Activity coefficient methods (9 models)

Special data packages (5 models)

Henry's Law for noncondensibles model

Full combinations of VLE, LLE, and VLLE thermodynamics models

Transport property models

ASPEN PLUS

There are 74 thermodynamic property models grouped in 10 classes including:

Equations of state (15 models)

Fugacity coefficient correlations (4 models)

Activity coefficients (10 models)

Molar volume (11 models)

Enthalpy/free energy/entropy (13 models)

Vapor pressure (5 models)

Vapor liquid equilibrium ratio (4 models)

Henry's constant (2 models)

Complex solids density (2 models)

Complex solids enthalpy (8 models)

There are 25 transport property models grouped in four classes:

Thermal conductivity (8 models)

Surface tension (4 models)

Viscosity (9 models)

Diffusion coefficient (4 models)

CHEMCAD

There are 48 thermodynamic property models grouped in eight classes including:

Equation of state (9 models)

Activity coefficient methods (13 models)

Liquid density methods (4 models)

Empirical methods for K-values (3 models)

Special systems for K-Values (5 models)

User supplied K-Values (5 models)

Vapor pressure methods (3 models)

Enthalpy/entropy (6 models)

There are 13 transport property models grouped in three classes:

Viscosity (9 models)

Thermal conductivity (2 models)

Surface tension (2 models)

Maximum Size of Flow Sheet That Can Be Simulated

For all practical purposes, neither PRO/II, ASPEN PLUS nor CHEMCAD have any limit on the maximum size of a flowsheet that can be simulated. This means there is effectively no limit to the number of unit operations, component streams, or recycles that can be included in a flowsheet model.

Number and Types of Convergence Algorithms Available for Recycle Calculations

The presence of recycle streams (return of all/part of material from an up-stream unit to a down-stream unit) in a flowsheet model creates a situation where the flow rate and composition of the recycle stream must be known first in order to carry out the calculation on the down-stream unit. This requires that a guess be made of the recycle stream (a feed to the down-stream unit) and then compared to the resulting calculations done at the up-stream unit. If the guessed and calculated values are "acceptably" close, the recycle stream is said to be converged. If not, the calculated values are used in some way to create the next guess. A convergence algorithm implements this procedure with the user having control over the maximum number of iterations and the convergence tolerance.

PRO/II

PRO/II contains three convergence algorithms for recycle calculations. These are Wegstein, Direct Substitution, and Broyden.

ASPEN PLUS

ASPEN PLUS has seven convergence algorithms for recycle calculation. These are Wegstein, Direct Substitution, Secant, Newton, Broyden, Complex, and Sequential/Quadratic Programming.

CHEMCAD

CHEMCAD has four convergence algorithms for recycle calculations. These are Direct Substitution, Wegstein, Dominant Eigenvalue Method, and Newton.

Model Debugging Features

PRO/II, ASPEN PLUS, and CHEMCAD have no special debugger program, but accomplish debugging by using expert systems, running the software interactively, adding each unit operation modularly until all the unit operations run without error.

Repetitive Run and Case Study Capabilities

PRO/II, ASPEN PLUS, and CHEMCAD can run various sets of data serially, one after the other. In addition, for a given set of input some or all the unit operations models can be run.

Built-In Optimization Algorithms

PRO/II and ASPEN PLUS have built-in optimization algorithms that will repetitively run a process simulation until an extremum for a given objective function (specified by the user) is found.

PRO/II

PRO/II contains a built-in second order constrained optimization algorithm.

ASPEN PLUS

A process design my be optimized by manipulating feed streams and/or block input variables. Equality or inequality constraints may be imposed on the optimization. The objective function and the constraint functions may be any flowsheet variables the user designates or may be a function of flowsheet variables computed using FORTRAN expressions or in-line FORTRAN statements. Optimization problems must be solved iteratively. By default, ASPEN PLUS will automatically generate and sequence a convergence block for the optimization problem, or the user may enter his own convergence specifications.

Two optimization algorithms are available in ASPEN PLUS: the COMPLEX method and Sequential Quadratic Programming (SQP) method. The COMPLEX method uses a simple "black-box" pattern search. The method can handle inequality constraints and bounds on decision variables. The COMPLEX method frequently takes many iterations to converge, but does not require numerical derivatives. It has been widely used for all kinds of optimization applications for many years and offers well-established and reliable option for optimization convergence.

The SQP method is a state-of-art quasi-Newton nonlinear programming algorithm that can converge tear streams, equality constraints, and inequality constraints simultaneously with the optimization problem. The SQP method usually converges in only a few iterations, but requires numerical derivatives with respect to all decision and tear variables at each iterations.

The SQP method as implemented in ASPEN PLUS includes a novel feature in which the tear streams can be partially converged using Wegstein during each optimization iteration and during line searches. This usually stabilizes convergence and can reduce the overall number of iterations. The user can specify the number of Wegstein passes. Choosing a large value effectively makes SQP a feasible path (but not a black-box) method.

The default optimization convergence procedure in ASPEN PLUS is to converge tear streams and the optimization problem simultaneously using the SQP method.

CHEMCAD

CHEMCAD does not offer built-in optimization algorithms at this time. However, in combination with the case study feature, the user could write his own optimization routine (in FORTRAN or C) which would run at the end of each case trial, evaluate the objective function, and choose values of the independent variable for the next trial case.

Standard Report Generation (Text and Graphics)

PRO/II, ASPEN PLUS, and CHEMCAD have standard report generation capabilities for generation of text and graphics.

Hardware Requirements

PRO/II

IBM 486 PC or compatible
Minimum of eight megabytes extended memory
Minimum of 60 megabytes free hard disk space
VGA monitor

ASPEN PLUS

IBM 386, 486, or compatible
Eight megabytes of extended memory
Math coprocessor (for 386)
VGA monitor
Minimum of 50 megabytes free hard disk space

CHEMCAD

IBM XT, AT,386,486 or compatible
580 K DOS memory or four megabytes of extended memory
Math coprocessor (for 386 and below)
CGA, EGA, VGA or compatible screen
Minimum of 15 megabytes of free hard disk space

Operating System Requirements/Limitations

PRO/II

Windows 3.1 in 386 enhanced mode and MS DOS 4.01 or higher.

ASPEN PLUS

MS DOS 5.0 or higher

CHEMCAD

MS DOS 3.0 or higher.

Network Implementability

Network versions of PRO/II, ASPEN PLUS, and CHEMCAD are available for installation in a client/server environment.

Future Upgrade for Dynamic Analysis

PRO/II

PRO/II at this time does not have an upgrade for dynamic analysis. However, a dynamic simulation product that will use the same graphics interface that is used in PRO/II is currently under development.

ASPEN PLUS

Aspen Technology Inc. offers a program called SPEEDUP which does dynamic simulation. This is a separate program from ASPEN PLUS and can be leased for an additional fee. SPEEDUP is compatible with ASPEN PLUS and thus the data from SPEEDUP can be imported to ASPEN PLUS or visa-versa. The two programs can be run sequentially to study a process for steady state and dynamic results for a given set of input parameters.

CHEMCAD

CHEMCAD at this time does not have an upgrade for dynamic analysis, although a new version to be released at the end of 1994 will have limited dynamic capabilities.

Types of Processes That Can Be Handled

Physical property models, data, and unit operation models are the key to obtaining useful simulation results, allowing the user to select the most appropriate model for the process to be simulated. The types of processes that can be handled will depend on these libraries. As has been discussed in the previous paragraphs, PRO/II, ASPEN PLUS, and CHEMCAD all have extensive libraries and, in general, can simulate a multitude of continuous steady state processes, with options for selected batch unit operations, e.g., reactors, distillation.

PRO/II

PRO/II evolved from a flowsheet simulation system known as PROCESS, which specialized in refinery operations. As such, PRO/II has retained a very strong refinery process simulation capability. In addition, it can handle a wide range of organic and inorganic processes such as production of ammonia and industrial gases, petrochemicals, and electrolytic systems such as amines, acids, salts, sour water, and caustic scrubbing. PRO/II can rigorously model complex electrolyte chemistry, non-ideal distillation, a wide variety of reactive systems, and vapor/liquid/solid separation. PRO/II includes unit operations to handle both organic and inorganic solids formation and separation for a variety of chemical processes.

ASPEN PLUS

ASPEN PLUS can handle a broad range of organic and inorganic processes, including chemicals, petrochemicals, and refining. ASPEN PLUS handles solids and complex substances such as polymers, wood pulp, coal, inorganic salts, and minerals. ASPEN PLUS has an extensive data library and equation base for electrolytes employing state-of-the-art computational techniques. Recent unit operation models for waste treatment processes which handle biomass and sludge have been added.

CHEMCAD

CHEMCAD, like ASPEN PLUS and PRO/II, can model processes with solids and electrolytes as well as organic and inorganic processes.

Cost Analysis

PRO/II

Data may be ported to an economic evaluation program like ICARUS (design costing package for chemical process flow sheets).

ASPEN PLUS

ASPEN PLUS does a crude costing analysis (+/-20%) for a given design. However, for a more precise analysis, data may be ported to a costing package like ICARUS.

CHEMCAD

Data may be ported to an economic evaluation program like ICARUS.

Statistical Capabilities

PRO/II, ASPEN PLUS, and CHEMCAD have the usual statistical packages for performing data regression and optimization.

PRO/II

PRO/II's regression program can fit experimental pure component and mixture data to a variety of equation forms, including any PRO/II correlation that has adjustable parameters.

ASPEN PLUS

ASPEN PLUS's Data Regression System (DRS) generates physical property model parameters using data from the literature or the laboratory. DRS handles all kinds of data for any number of components. DRS fits parameters of any models in any combination.

CHEMCAD

CHEMCAD uses regression methods to generate physical properties of pure components, multiple components for VLE and LLE, UNIFAC, and infinite dilution data.

Customer Support

PRO/II, ASPEN PLUS, and CHEMCAD have customer support organizations that offer training courses and consulting.

PRO/II

SimSci provides customer support services as part of a client's lease arrangement. SimSci offers training seminars regularly for every level user at a number of locations worldwide.

ASPEN PLUS

Aspen Tech maintains worldwide offices staffed with full-time engineers dedicated to technical support. Questions can be submitted by telephone hot lines, telefax, telex, or computer link. On site assistance is available. Training courses are offered regularly. In-house courses are offered tailored to the customer's needs.

CHEMCAD

Chemstations provides training and consulting on a regular basis. Questions can be submitted by telephone hot line, telefax, or computer link.

Potential Dual Use Capability

PRO/II, ASPEN PLUS, and CHEMCAD can be used both by government laboratories/technical centers and private industry. Since the software runs on commonly available PC platforms, models developed either at government or commercial sites can be easily transferred and shared provided both sites have the same simulation software package and any restrictions due to security classification and/or proprietary data have been accommodated.

EVALUATION OF FEATURES

An effort has been made to rate and compare each of the three software packages by assigning a numerical value of 1 to 10 (based on assessment of importance) to each characteristic/attribute in table 1 (excluding cost) and scoring each package from 1 (low) to 5 (high). The individual feature scores were then added and subsequently divided by the total value of all features to give a final percent rating. Unfortunately, there is no absolute way to do this. The rating methodology is subjective, both in the weighing of characteristics and, more significantly, in the scoring for each software package. The numbers are based solely on the expertise and over 20 years working experience of the authors as chemical process simulation practitioners, which it is assumed the reader will consider when assessing the results. By this methodology, it is seen that based on features/attributes/capabilities, ASPEN PLUS is the highest rated package with CHEMCAD second and PRO/II third. The rating matrix is shown in table 2.

An attempt has also been made to factor in cost by assessing performance versus price. A simplistic price/performance index can be computed by dividing the performance rating (%) by annual cost ($K) for a single year of software use. By this method, using the first year costs of $25.0, $24.0 and $11.5 for PRO/II, ASPEN PLUS, and CHEMCAD, respectively, price/performance indices of 3.13, 3.80, and 6.91, respectively, were computed. Thus, it would appear that CHEMCAD offers significantly better value, which increases over time since the CHEMCAD annual maintenance fee is much less than either PRO/II's or ASPEN PLUS's leasing fee.

CONCLUSIONS

1. PRO/II, ASPEN PLUS, and CHEMCAD are all very similar in form, function, look, and feel, with each providing a highly structured, graphically interfaced software system having the capability to simulate virtually any large size chemical manufacturing process.

2. Each has certain strengths and weaknesses, with ASPEN PLUS excelling in the areas of solids handling, electrolytic process simulation, and use of expert system technology; PRO/II having the best capability for refinery simulation; and CHEMCAD offering the best graphical user interface.

3. Overall, based on the aggregate score for all the criteria chosen for evaluation, ASPEN PLUS is rated highest.

4. When cost is factored in, CHEMCAD stands out as the best value.

5. Assuming the availability of file-linking software, each of the three simulation packages could be interfaced with a larger life cycle modeling system.

RECOMMENDATIONS

1. In a situation where stand-alone chemical process flowsheet simulation is to be carried out and an annual resource outlay on the order of $25,000 is not considered prohibitive, ASPEN PLUS should be used.

2. As a detailed chemical process simulation tool used in the broader context of a life cycle modeling system where many of the stand-alone features would not routinely come into play, CHEMCAD should be chosen because of its acceptable performance, its superior cost/performance ratio and its underlying C code (which would likely make integration into the larger system easier).

Table 1
Characteristics/attributes for software package evaluation

- Purchase Cost and/or Licensing Requirements
- Number and Type of Different Unit Operation Models
- Extent of Detail in Unit Operation Models
- Quality and Features of Graphical Interface
- Ease of Simulation Creation
- User Friendliness and Expected Learning Curve Time
- Open Architecture
- Extent of Vendor-Supplied Physical Properties Databases and Ability to Link New Databases and/or Compounds
- Number and Type of Thermodynamic and Physical Property Models
- Maximum Size of Flow Sheet That Can Be Simulated.
- Number and Type of Convergence Algorithms Available for Recycle Calculations
- Model Debugging Features
- Repetitive Run and Case Study Capabilities
- Built-In Optimization Algorithms
- Standard Report Generation(Text and Graphics)
- Hardware Requirements
- Operating System Requirements/Limitations
- Network Implementability
- Future Upgrade for Dynamic Analysis
- Types of Processes That Can Be Handled
- Cost Analysis Capabilities
- Statistical Capabilities
- Customer Support
- Potential "Dual Use" Capability

Table 2
Evaluation matrix for flowsheet simulation software systems

FEATURE	VALUE	Rating 1-5 (Low to High) PRO/II	ASPEN	CHEMCAD	SCORE PRO/II	ASPEN	CHEMCAD
Number and Type of Different Unit Operations Models	10	4	5	4	8	10	8
Extent of Detail in Unit Operation Models	10	4	4	4	8	8	8
Quality and Features of the Graphical User Interface	8	4	4	5	6.4	6.4	8
Ease of Simulation Creation	8	4	4	4	6.4	6.4	6.4
User Friendliness and Expected Learning Curve Time	5	4	5	5	4	5	5
Open Architecture	5	5	4	3	5	4	3
Extent of Vendor-Supplied Physical Properties Data Base(s) and Ability to Link New Data Bases and/or Compounds	10	4	5	4	8	10	8
Number and Type of Thermodynamic and Transport Property Models	8	3	5	4	4.8	8	6.4
Maximum Size of Flow Sheet That Can Be Simulated	8	5	5	5	8	8	8
Number and Type of Convergence Algorithms Available For Recycle Calculations	5	3	5	4	3	5	4
Model Debugging Features	8	3	5	4	4.8	8	6.4
Repetitive Run and Case Study Capabilities	5	5	5	5	5	5	5
Built - In Optimization Algorithms	6	3	5	0	3.6	6	0
Standard Report Generation (Text and Graphics)	6	5	5	5	6	6	6
Hardware Requirements	3	3	4	5	1.8	2.4	3
Operating System Requirements/ Limitations	3	3	4	5	1.8	2.4	3
Network Implementability	5	4	4	4	4	4	4
Future Upgrade for Dynamic Analysis	5	3	4	3	3	4	3
Types of Processes That Can Be Handled	8	4	5	3	6.4	8	4.8
Cost Analysis Capabilities	8	4	5	4	6.4	8	6.4
Statistical Capabilities	5	4	4	4	4	4	4
Customer Support	10	4	4	4	8	8	8
Potential "Dual Use" Capability	5	4	4	4	4	4	4
TOTAL	154				120.4	140.6	122.4
OVERALL RATING (%)					78.18	91.30	79.48

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